

Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-
26946-56-5 | DTXSID10447169

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.83e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.34e-01

Confidence level: 6.47e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Octadecanethiol</div> <div>Measured: 1.02</div> <div>Predicted: 1.14e-06</div>	<div>Image not found</div> <div>2,4-D, Dimethylamine salt</div> <div>Measured: 1.30e-02</div> <div>Predicted: 7.12e-07</div>	<div>Image not found</div> <div>Benzene, octyl-</div> <div>Measured: 5.60e-03</div> <div>Predicted: 1.26e-02</div>
<div>Image not found</div> <div>2,4-D-Butotyl</div> <div>Measured: 1.04e-02</div> <div>Predicted: 8.01e-06</div>	<div>Image not found</div> <div>2,2-Dimethylheptane</div> <div>Measured: 8.85e-02</div> <div>Predicted: 9.39</div>	